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An improved convergence criterion based on normalized residual for heat transfer and fluid flow numerical simulation

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ABSTRACT

In the numerical simulation of heat transfer and fluid flow problems, residual is often adopted as a convergence criterion. Since residual is susceptible to several factors, such as the property of physical problems, the expression form of discretized equations, the scale of grid and the nondimensionalization of governing equations, the converged value differs greatly in different cases. Thus, it is hard to set a specific residual value in a specific numerical calculation. To give a universal convergence criterion in this paper, a residual based on normalization idea is proposed. Range of specified values of this improved convergence criterion for general heat transfer and fluid flow problems is also given in this paper. Numerical simulation results indicate that the improved convergence criterion based on normalized residual is much more reasonable than the one based on traditional residual.

1. Introduction

In the field of numerical heat transfer and computational fluid dynamics (NHT & CFD), iterative methods, such as Gauss–Seidel (GS), preconditioned conjugate gradient (PCG), generalized minimal residual (GMRES), are widely used in the solution of large scale algebraic equations which arise from discretized partial differential equations. To reduce the iterative error and save the computational cost, convergence criterion in the iterative calculations should be reasonably defined. Stopping iterations prematurely may lead to inaccurate solutions which do not reach to prescribed accuracy while prolonged iterations may increase computational expense without proportionate gain in accuracy. A reasonable convergence criterion should show a good balance between iterative error and computational time, and it should also reflect the convergence behavior of calculation process correctly.

In 1993, the Journal of Fluids Engineering defined a list of guidelines for the control of numerical accuracy. One of them is that: stopping criteria for iterative calculations need to be precisely explained and estimates must be given for the corresponding convergence error [1]. After that, many researches focused on this issue. For instance, Coleman et al. [2] developed a new approach to CFD code validation and defined the comparison error as the difference between the data and simulation values. The convergence criterion for validation is that the magnitude of the comparison error must be less than the validation uncertainty. Roache [3] studied the grid convergence systematically and gave a list of journal policy statements on control of numerical accuracy in the appendix. Freitas [4–5] reviewed the status of methods for evaluation of numerical uncertainty and pointed out the grid independence or convergence must be established and iterative convergence criteria must be addressed where appropriate. Axelsson et al. [6] presented some estimates on the lower and upper bounds for the PCG iteration errors measured both on energy norm and Euclidean norm, which can be used as convergence criteria. Smith et al. [7] used the relative improvement norm as convergence criterion for Krylov iterative methods, the numerical analyses indicate that the convergence criterion only depends on the approximate solutions. Najafi et al. [8] proposed a new computational GMRES method, in which the residual norm was adopted as the convergence criterion. Chen et al. gave several popular convergence criteria in [9], such as relative residual norm and relative improvement norm, which are frequently used in practice finite element method (FEM) for symmetric positive definite linear system and the symmetric indefinite system. It was pointed out that the relative improvement norm must be adopted with great care in symmetric indefinite system. Though the selection of convergence criterion is significant to control numerical accuracy and computation

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Nomenclature

a_0, a_i	coefficients in the discretized equation
a_0^*, a_i^*	dimensionless coefficients
$\tilde{a}_0$, $\tilde{a}_i$	normalized coefficients
b_0	source term in the discretized equation
b_0^*	dimensionless source term
$\tilde{b}_0$	normalized source term
l	side length of computational domain, m
N_{grid}	grid number
p	pressure, Pa
P	dimensionless pressure
Re	Reynolds number
$\tilde{res}$	normalized residual
$\tilde{res}_{ave}$, $\tilde{res}_{max}$	average and maximum absolute values of normalized residual
$\tilde{S}$	source term in dimensionless governing equation
u, v	velocity components in x and y coordinate directions, m/s
u_{top}, U_{top}	dimensional and dimensionless lid-driven velocity
U, V	dimensionless velocity components in X and Y coordinate directions
x, y	coordinates in x and y directions
X, Y	dimensionless x and y

Greek symbols

ε_1, ε_2	specified value of convergence criterion
ϕ_{P_0}, ϕ_i	variables
$\phi_{P_0}^*$, ϕ_i^*	dimensionless variables
$\tilde{\phi}_{P_0}$, $\tilde{\phi}_i$	normalized variables
ΔV	control volume
ς, η	ratios generated in the nondimensionalization of governing equation
λ	heat conductivity coefficient, W/(m.°C)
μ	dynamic viscosity, Pa s
ρ	density, kg/m^3
Γ_ϕ	general diffusion coefficient

Subscripts

ave	average
grid	grid
i	number of the adjacent nodes
max	maximum
P_0	interested node number
top	top
N, S, W, E	north, south, west, east

Superscripts

*	dimensionless

Prefixes

∇	gradient

expense, consensus has not been reached for how to set the convergence criterion reasonably and scientifically in the heat transfer and fluid flow numerical simulation [10].

Residual can be easily obtained and directly reflects the differences between numerical solutions and true solutions, therefore it has been frequently adopted as a convergence criterion in the field of NHT&CFD [11–15]. The most commonly used convergence criteria are as follows: (1) maximum value or norm of residual [16]. When the maximum value or norm of residual is no more than a specified value, calculation is seemed to be converged; (2) decrease rate of residual (relative residual) [17]. When the decrease rate of residual is no more than a specified value, calculation is seemed to be converged; (3) relative error of residual or characteristic quantity [18]. When the change of relative error of residual or characteristic quantity in some iterative steps is no more than a specified value, calculation is considered as converged.

Nevertheless, analyses on the above common convergence criteria indicate that all of them have their own limitations: (1) maximum value and norm of residual are both absolute quantities which are greatly influenced by the types and properties of physical problems. In addition, different expression forms of discretized equations can be obtained from the same governing equation according to personal preference. In this way, it is difficult to judge the convergence condition for the calculation when an absolute quantity is adopted as convergence criterion. (2) relative residual can overcome the disadvantage of maximum value or norm of residual. However, this criterion is easily affected by the initial field. When the initial field is close to the true solution, the decrease rate of residual would keep a constant around 1.0, which may be larger than the specified value and results in the failure of convergence judgment. (3) under-relaxation strategy is often utilized because research objectives of heat transfer and fluid flow numerical simulation are usually non-linear physical problems. If the under-relaxation factor is set as a very small value, change of variables in some iterative steps can be relatively small. Thus, selecting relative error of residual or characteristic variable as convergence criterion is not reasonable enough as well. Besides, it is found that in some problems, the calculation has converged when residual is less than the magnitude of 10^{-6} while in some others, the converged solution has still not been obtained even when residual is less than the magnitude of 10^{-12}. Even for the same physical problem where all calculation conditions are the same except for the grid density, to obtain the solution with same prescribed accuracy, the specified value for convergence criterion may differ from each other in a gap of several orders of magnitude.

Therefore, adopting residual as convergence criterion in the numerical calculation is not reasonable enough. Residual is influenced by several factors and its value range varies greatly, which makes it difficult to set a specified value for different sorts of problems. Based on this, the present paper conducts a preliminary study on the selection of convergence criterion and setting of specified value as convergence criterion in the numerical calculation of heat transfer and fluid flow problems. An improved convergence criterion based on normalized residual is proposed.

The structure of this paper is organized as follows: In Section 2, factors influencing the value of residual are analyzed from several aspects, such as physical problem property, expression form of discretized equations, grid scale and nondimensionalization of governing equations. In Section 3, an improved convergence criterion based on normalized residual focused on the factors mentioned above is proposed. Reference range of specified value for the proposed convergence criterion in general heat transfer and fluid flow problems is also presented in this section. In Section 4, convergence criteria based on normalized residual and traditional residual respectively are concretely analyzed and compared by